Numerical Simulation of Influence Parameters during Droplet Generation in a Microfluidic T-junction

Wei Wei1,2, Fang Wu1
1Tianjin Key Laboratory for Control Theory and Applications in Complicated System
Tianjin University of Technology
391, Binshui Xidao, Xiqing District, Tianjin, 300384, China
weiwei@tjut.edu.cn

Shuxiang Guo1,3, Jian Guo1,2
2Biomedical Robot Laboratory
Tianjin University of Technology
391, Binshui Xidao, Xiqing District, Tianjin, 300384, China
wf8023zly@163.com

Yuehui Ji1,2, Xu Ma1,2
Kagawa University
2217-20, Hayashi-cho, Takamatsu, 761-0396, Japan
guo@eng.kagawa-u.ac.jp

Abstract - Droplets had a significant advantage that each droplet could be regarded as an individual chemical reactor. However, the microchip for droplets generation was very difficult to design. Numerical simulation was done in order to provide a theoretical basis for microchip design. This paper described a three-dimensional numerical simulation on droplets behavior in a microfluidic T-shaped based on volume-of-fluid (VOF) model. The wetting property, the velocity and viscosity of continuous phase, the surface tension between two phases and the size of microchannel had been analyzed, which impacted the droplets' behavior. Droplets can be generated when the contact angle was set from 0 degree to 90 degrees. With the velocity and viscosity of continuous phase increasing, droplets diameter would decrease gradually. The diameter of droplets increased according to the improvement of the surface tension between two phases. The droplets diameter was found to exhibit a linear dependence on the microchannel size. This work would contribute to the design of droplet microchips for better biochemical analysis, pharmaceuticals and so on.

Index Terms - Microfluidic systems, Numerical simulation, Volume-of-fluid (VOF) model, T-shaped, Microchip design

I. INTRODUCTION

Microfluidic systems have possessed a broad range of applications in chemical [1], biological [2], medical [3] and environmental analysis [4]. Microfluidic systems can be divided into the continuous flow microfluidic systems and the droplet-based microfluidic systems. Droplet-based microfluidic systems can avoid cross-contamination because droplet acted as an individual chemical reactor. In general, the size of a single droplet is $10^{-15} - 10^{-9}$L, less sample or reagent is consumed. Chemical reaction is faster because of circulating reflux which is formed in the droplet. The volume of droplet is controlled by means of adjusting micropump. There has been growing interest in droplet-based microfluidic systems because of these advantages.

It is obvious that droplet-based microfluidic systems have lots of advantages. Nevertheless the droplet is formed in the microchannel of the microchip. It is very difficult to design a microchip for droplets generation because there are too many factors affecting the droplet generation, such as the wetting property, the velocity of continuous phase, the viscosity of continuous phase, the interface tension between continuous phase and disperses phase, and the size of microchannel. How these parameters affect droplets generation and which parameter or even several parameters is the major effect factor in the process of droplets generation. Microchips are designed failure on the basis of we know nothing about influence factors. It can be concluded that an adequate cause is required to design a microchip. The scene of droplets generation can reproduce and the situation of droplet change with influence factors by numerical simulation. There is almost no difference between simulation and experiment results. Thus numerical simulation can provide theory evidence to design a microchip.

There are lots of researches about numerical simulation of droplets in a fairly recent historical survey. In 2009, Liu et al. has used a 2D model to investigate the behavior of microdroplets flowing in microchannels with a series of diffuser structures [5]. In 2010, Gupta and Kumar have investigated the dependence of velocity of the continuous and dispersed phases on the length of the droplets formed [6]. In 2012, Yan et al. has simulated various droplet flow patterns such as long slugs, small spheres, stable stream and parallel flows. In that paper, the pressure of the junction point fluctuated as a new parameter is considered [7]. In 2013, Guillaumet et al. has described a two dimensional simulation of segmented micro co-flows of CO2 and water in micro-capillaries. The effects of the wetting property of the capillary walls and the interfacial tension between CO2/water are described [8]. These computational works were validated by comparing numerical and experimental results. The simulation results demonstrate that the process of the droplets generation in the immiscible liquids can be reasonably predicted and it can provide a theoretical basis for chip design.

Based on our previous work, the droplet size is detected to realize the droplet-based microfluidic system more controllable. The size and volume of droplets are obtained by image processing and the results shown that microfluid can be controlled in quantitative [9]. Under certain circumstances, images are collected by image acquisition system has severe noise. Denoising is the most important step and the effect of denoising can affect the further steps. A new denoising method based on wavelet threshold function is proposed to improve image quality [10]. In this paper, we focus on the model of T-shaped microchannel for droplets generation. The droplet-based microchips which designed in optimum material and size based on simulation results.
II. CALCULATION MODEL AND PARAMETERS

In this paper, a T-shaped microchannel is built to simulate the droplet behavior. The model of the T-shaped microchannel in this simulation is shown in Fig.1. In this simulation, a constant T-shaped model is used when the wetting property, the velocity and viscosity of continuous phase and the surface tension between two phases are simulated to understand the process of droplet generation (as shown in Fig.1). The width and the thickness of the model are both 100um. The length of microchannel is 1000um. The size of microchannel is changed in order to illustrate the influence of the size of microchannel on droplet generation. Here, Fluid 1 is set as the continuous phase and Fluid 2 is set as the disperse phase. Fluid 2 enters through the vertical channel, the other fluid, Fluid 1, flows from the left to right through the horizontal channel. Customarily, Fluid 1 and Fluid 2 are immiscible liquids such as water and oil.

\[ F = -\sigma k V \phi \]  \hspace{1cm} (5)

where \( \sigma \) and \( k \) are the surface tension and surface curvature, respectively. The surface curvature can be calculated by:

\[ k = \nabla \cdot \frac{V \phi}{|V \phi|} \]  \hspace{1cm} (6)

In order to solve the equation (1), (2) and (3), boundary conditions are set as follows. In the T-shaped microfluidic, heat exchange can be ignored. At both inlets, Laminar inflow conditions with prescribed volume flows are used. The velocity of continuous phase and disperse phase is constant. \( v_1 \), as well as \( v_2 \), represents the velocity of continuous phase and disperse phase, respectively. At the inlet to the continuous phase, the velocity \( v_1 \) only has horizontal component and the value of volume fraction is set as \( \phi = 1 \). Likewise, at the inlet to the disperse phase, the velocity \( v_2 \) only has vertical component and the value of volume fraction is set as zero \( (\phi = 0) \). The outlet of the flow channel is set as outlet boundary condition, where atmospheric pressure was used, \( P_{atm} = P_{atm} \). The wetting boundary condition was applied at the wall of flow channel with the contact angle and a slip. The contact angle is the angle between the fluid interface and the solid wall at points where the fluid interface attaches to the wall. The slip length is the distance to the position outside the wall where the extrapolated tangential velocity component is zero.

The effective diameter of droplet can be obtained using the following expression:

\[ d_{eff} = \frac{3}{4\pi} \int_{\Omega} \frac{1}{2} (\phi > 0.5) d\Omega \]  \hspace{1cm} (7)

where \( d_{eff} \) is the effective diameter of droplet, \( \Omega \) represents the leftmost part of the horizontal channel.

B. Parameters

Droplet generation requires strict conditions. It is influenced by some parameters, for instance, the wetting property, the velocity of continuous phase, the viscosity of continuous phase, the surface tension between two phases and the size of microchannel. Droplet is controlled by these parameters. The volume of droplet has been calculated using Lattice Boltzmann Method (LBM) proposed by Van der Graaf et al. [12]. It is expressed as:

\[ V = V_{crit, ref} C_a^{n_1} + t_{neck, ref} C_a^{n_2} \phi_d \]  \hspace{1cm} (8)
where \( Ca \) is the capillary number which describes the relative of the viscosity and the interfacial tension, \( V_{\text{crit}, \text{ref}} \) is the critical volume at \( Ca = 1 \) and \( t_{\text{neck}, \text{ref}} \) is the necking time at \( Ca = 1 \), \( m \) and \( n \) are constant, \( \phi_e \) is the to-be-dispersed phase flow rate. The capillary cumber is an essential parameter to effect droplet generation. It is defined as:

\[
Ca = \frac{\mu \nu_e}{\sigma}
\]

(9)

where \( \mu \) is the viscosity of continuous phase, \( \nu_e \) is the velocity of continuous phase, \( \sigma \) is the surface tension coefficient between continuous phase and disperse phase. In order to introduce the size of microchannel has an influence on droplet generation. The two non-dimensional numbers are introduced, namely, Reynolds number (\( Re \)) and Weber number (\( We \)). They are set as:

\[
Re = \frac{\rho v_0 D_H}{\mu}
\]

(10)

\[
We = \frac{\rho v_0^2 D_H}{\sigma}
\]

(11)

where \( v_0 \) is the average velocity, \( D_H \) is the equivalent diameter of cross-sectional of microchannel. The Reynolds numbers is the ratio of the influence of viscous force to the inertia force. The Weber number determines the influence of inertia force compared to the surface tension force. The size of microchannel determines the influence of the Reynolds numbers and the Weber number. But in microscopic field, scale effect is existed. The effect of microchannel size on droplet generation is very difficult to predict.

The droplet is broken off from the microchannel walls during droplet generation. The wetting property of microchannel is one of the factors that cannot be ignored. The goal that the wetting property change of the dispersed phase microchannel walls without other properties changing is not achieved rely on experiment simply. As a result, the wetting property is not studied systematically [13]. In simulation, the wetting property is studied by setting wall contact angle [14]. Young's law gives the relation between a contact angle and interfacial tensions. For a W-O-W droplet, the contact angle is written as:

\[
\cos(\theta) = \frac{\sigma_{w, \text{wall}} - \sigma_{o, \text{wall}}}{\sigma_{ow}}
\]

(12)

where \( \sigma_{w, \text{wall}} \) is the interfacial tension of water with the surface, \( \sigma_{o, \text{wall}} \) is the interfacial tension of oil with the surface, and \( \sigma_{ow} \) is the interfacial tension of the oil/water interface. In the simulation, the contact angle between the fluid and the wall surface is changed by adjusting the surface normal of the unit near the wall. The surface normal of the unit can be expressed as follows:

\[
\hat{n} = \hat{n}_w \cos \theta + \hat{t}_w \sin \theta
\]

(13)

where \( \theta \) is the contact angle, \( \hat{n}_w \) and \( \hat{t}_w \) are the unit normal vector and the unit tangent vector of the wall, respectively.

In order to testify the accuracy of the simulation, parameters are defined the same as Van der Graaf [12]. The densities of two fluid are set as 1.00×10^3 Kg/m^3 and 1.02×10^3 Kg/m^3 with the dynamic viscosities of 1.95×10^{-3} Pa.s and 6.71×10^{-3} Pa.s, respectively. The value parameters is set based on two liquids that is 1,6-hexanediol diacrylate and a 2wt% poly (vinyl alcohol) aqueous solution. The surface tension is set as 5×10^{-3} N/m. The velocity of the continuous phase and the dispersed phase are set as 4×10^{-7} m^3/h and 2×10^{-7} m^3/h, respectively. The simulation result of droplet generation is shown in Fig. 3 can fit with the experimental results obtained by Van der Graaf.

A. The Wetting Property

The wetting property is the contact angle between the fluid and the wall surface. The wetting property is changed by the contact angle which is set as 0° to 90°. Interval is 5°. The other parameters are set as TABLE I.

<table>
<thead>
<tr>
<th>TABLE I</th>
<th>PARAMETERS OF THE SURFACE TENSION SIMULATION</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>The continuous phase</td>
</tr>
<tr>
<td>Viscosity</td>
<td>1.95×10^{-3} Pa.s</td>
</tr>
<tr>
<td>Density</td>
<td>1002Kg/m^3</td>
</tr>
<tr>
<td>Surface Tension</td>
<td>5×10^{-3} N/m</td>
</tr>
<tr>
<td>Contact Angle</td>
<td>variety</td>
</tr>
<tr>
<td>Flow rate</td>
<td>4×10^{-7} m^3/h</td>
</tr>
<tr>
<td>Microchannel size</td>
<td>100×100μm</td>
</tr>
</tbody>
</table>
The contact angle at $\theta = 0^\circ$ (a) The contact angle at $\theta = 30^\circ$ (b) The contact angle at $\theta = 60^\circ$ (c) The contact angle at $\theta = 90^\circ$ (d) The contact angle at $\theta = 90^\circ$

Fig. 4 The effect of the wetting property for droplet

The partial results of simulation are shown in Fig. 4. The results show the droplet cannot be generated when the contact angle is bigger than 90°. In the condition of other parameters remained constant, the diameter of droplet increases gradually with the contact angle increases. Fig. 5 shows the relationship between the contact angle and the droplet diameter. The figure indicated that with the contact angle increase, the droplet diameter is found accretion.

Fig. 5 The relationship between the droplet diameter and the contact angle

B. The Velocity of Continuous Phase

In the simulation, the velocity of continuous phase is replaced by the flow rate of continuous phase. The flow rate equals to the product of velocity and cross-sectional area of microchannel. Parameters are set as TABLE II. The flow rate of continuous phase is varied from $1 \times 10^{-7}$ m$^3$/h to $1 \times 10^{-6}$ m$^3$/h.

![TABLE II](image)

Some examples of droplet generation in different flow rates are shown in Fig. 6. The shear force of continuous phase is accelerating when the velocity of continuous phase is increased and the velocity of dispersed phase keep constant. The time of droplet broken becomes shorter. Thus, the droplet diameter reduced while the velocities of continuous phase increasing (Fig. 7).

![TABLE III](image)

C. The Viscosity of Continuous Phase

In this part simulation, parameters are set as TABLE III. The viscosity of continuous phase is changed with $0.45 \times 10^{-3}$ Pa.s, $0.95 \times 10^{-3}$ Pa.s, $1.45 \times 10^{-3}$ Pa.s, $1.95 \times 10^{-3}$ Pa.s, $2.45 \times 10^{-3}$ Pa.s, $2.95 \times 10^{-3}$ Pa.s, $3.95 \times 10^{-3}$ Pa.s, $4.95 \times 10^{-3}$ Pa.s, $5.95 \times 10^{-3}$ Pa.s, $6.95 \times 10^{-3}$ Pa.s, $7.95 \times 10^{-3}$ Pa.s, $8.95 \times 10^{-3}$ Pa.s and $9.95 \times 10^{-3}$ Pa.s.

![Fig. 7](image)

Fig. 7 The relationship between the droplet diameter and the flow rate of continuous phase

Some examples of droplet generation in different flow rates are shown in Fig. 6. The shear force of continuous phase is accelerating when the viscosity of continuous phase is increased. The time of droplet broken becomes shorter.
D. The Surface Tension between Two Phases

In this part simulation, the surface tensions are set as $2.5 \times 10^{-3}$ N/m, $5 \times 10^{-3}$ N/m, $7.5 \times 10^{-3}$ N/m, $10 \times 10^{-3}$ N/m, $20 \times 10^{-3}$ N/m, $30 \times 10^{-3}$ N/m. The rest parameters are set as TABLE IV.

<table>
<thead>
<tr>
<th>TABLE IV PARAMETERS OF THE SURFACE TENSION SIMULATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>The continuous phase</td>
</tr>
<tr>
<td>Viscosity</td>
</tr>
<tr>
<td>Density</td>
</tr>
<tr>
<td>Surface Tension</td>
</tr>
<tr>
<td>Contact Angle</td>
</tr>
<tr>
<td>Flow rate</td>
</tr>
<tr>
<td>Microchannel size</td>
</tr>
</tbody>
</table>

The results of simulation are shown in Fig. 10. In the condition of other parameters remained constant, the diameter of droplet increases gradually with the surface tension increases. Fig. 11 shows the relationship between the surface tension and the droplet diameter.

E. The Size of Microchannel

In this part simulation, the parameters are set as TABLE V. In this model, the microchannel size is set as 100$\mu$m×100$\mu$m. In order to figure out the influence of the microchannel size, the microchannel size is are also set as from 110$\mu$m×110$\mu$m to 160$\mu$m×160$\mu$m. As we known, there is size effect in microfluidic. But size effect is not studied in the paper because the simulation is limited by computer. Smaller sizes of microchannel are simulated in this paper.

<table>
<thead>
<tr>
<th>TABLE V PARAMETERS OF THE SURFACE TENSION SIMULATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>The continuous phase</td>
</tr>
<tr>
<td>Viscosity</td>
</tr>
<tr>
<td>Density</td>
</tr>
<tr>
<td>Surface Tension</td>
</tr>
<tr>
<td>Contact Angle</td>
</tr>
<tr>
<td>Flow rate</td>
</tr>
<tr>
<td>Microchannel size</td>
</tr>
</tbody>
</table>

The results of simulation are shown in Fig. 12. The time of droplet generation is increased with the microchannel size. Fig. 13 shows the relationship between the microchannel size and the droplet diameter. It is clearly shown that the droplet diameter is linear with the microchannel size. The function is obtained by linear fitting. It can be expressed as follows:

$$d_{eff} = 1.5948h - 11.7132$$  \hspace{1cm} (14)

where $h$ is the size of microchannel.
The microchannel size was regulated by the micropump. The surface tension was influenced by some material of the continuous phase could change the viscosity of the continuous phase. The surface tension between two phases increased. The diameter of droplet kept a linear relationship with the length of the microchannel.

In microchip design, the wetting property was realized by modifier on the microchannel surface. The velocity of the continuous phase was similar to the velocity of the continuous phase. The relationship between the droplet diameter and the viscosity of the continuous phase was determined by requirement of experiment.

The simulation could not only provide theoretical basis but help experimenter to obtain droplets of a certain size by choosing different parameters.

In the future work, a microchip which is same as the model in this paper will be designed and manufactured to generate droplets. The microchip is used to do some experiment. The process of design is guided by simulation results in this paper.

ACKNOWLEDGMENT

This research is supported by Tianjin City High School Science & Technology Fund Planning Project (20120830).

REFERENCES